

Deferoxamine

70-51-9 | DTXSID7022887

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.77e-02 mol/L

Global applicability domain: Outside

Local applicability domain index: 2.48e-01

Confidence level: 5.13e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Deferoxamine</div> <div>Measured: 2.14e-02</div> <div>Predicted: 1.77e-02</div>	<div>Image not found</div> <div>Lisinopril</div> <div>Measured: 2.39e-01</div> <div>Predicted: 6.29e-02</div>	<div>Image not found</div> <div>Triamcinolone diacetate</div> <div>Measured: 7.42e-05</div> <div>Predicted: 5.87e-05</div>
<div>Image not found</div> <div>Hydrocortisone acetate</div> <div>Measured: 3.49e-05</div> <div>Predicted: 3.23e-05</div>		